LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082802.D
Acq On : 7 Nov 2015 11:05
Operator : UM/IZ
Sample : G4246-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12R

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.036	254	258	265	rVB	2384490	3533042	49.18%	5.295%
2	5.459	292	295	297	rBV	5822953	6721152	93.56%	10.072%
3	6.487	381	385	387	rVB	5365689	7184154	100.00%	10.766%
4	6.613	393	396	399	rBV	5528070	5911797	82.29%	8.859%
5	6.842	414	416	419	rBV	1384829	1579525	21.99%	2.367%
6	7.002	428	430	433	rBV	4545284	4415885	61.47%	6.618%
7	7.413	462	466	468	rBV	3557530	4570889	63.62%	6.850%
8	8.133	526	529	531	rBV	2498252	2217543	30.87%	3.323%
9	9.207	620	623	626	rBV	4729003	6401254	89.10%	9.593%
10	9.608	655	658	660	rBV	1908323	1744120	24.28%	2.614%
11	9.882	680	682	685	rBV	1789552	2480609	34.53%	3.717%
12	10.305	717	719	721	rBV	152170	141937	1.98%	0.213%
13	10.670	748	751	754	rBV	3928974	4406695	61.34%	6.604%
14	10.808	761	763	767	rVB	56623	90618	1.26%	0.136%
15	11.253	800	802	803	rBV2	96991	91797	1.28%	0.138%
16	11.368	809	812	814	rBV	2949970	2531097	35.23%	3.793%
17	11.676	837	839	841	rVV	87032	74494	1.04%	0.112%
18	11.905	857	859	864	rBV3	372089	604328	8.41%	0.906%
19	12.694	926	928	931	rBV	227144	245547	3.42%	0.368%
20	12.785	934	936	939	rVV	332717	363812	5.06%	0.545%
21	12.865	939	943	945	rVB2	79744	87686	1.22%	0.131%
22	12.956	948	951	954	rBV	5785641	5571440	77.55%	8.349%
23	13.494	996	998	1000	rBV	304517	264245	3.68%	0.396%
24	13.539	1001	1002	1007	rVB2	40517	73069	1.02%	0.109%
25	13.859	1028	1030	1040	rVB	374318	688211	9.58%	1.031%
26	13.997	1040	1042	1045	rBV	1822466	2348175	32.69%	3.519%
27	14.191	1056	1059	1065	rVB	59712	84929	1.18%	0.127%
28	14.499	1083	1086	1093	rBV2	84708	179880	2.50%	0.270%
29	14.762	1107	1109	1111	rBV	52753	86075	1.20%	0.129%
30	15.128	1138	1141	1142	rBV	49420	72026	1.00%	0.108%
31	15.425	1164	1167	1170	rBV	1129155	1739734	24.22%	2.607%
32	15.962	1211	1214	1225	rVB6	34221	140544	1.96%	0.211%
33	17.597	1354	1357	1360	rBV4	37954	84074	1.17%	0.126%

LSC Area Percent Report

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Acq On : 7 Nov 2015 11:05
Operator : UM/IZ
Sample : G4246-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12R

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

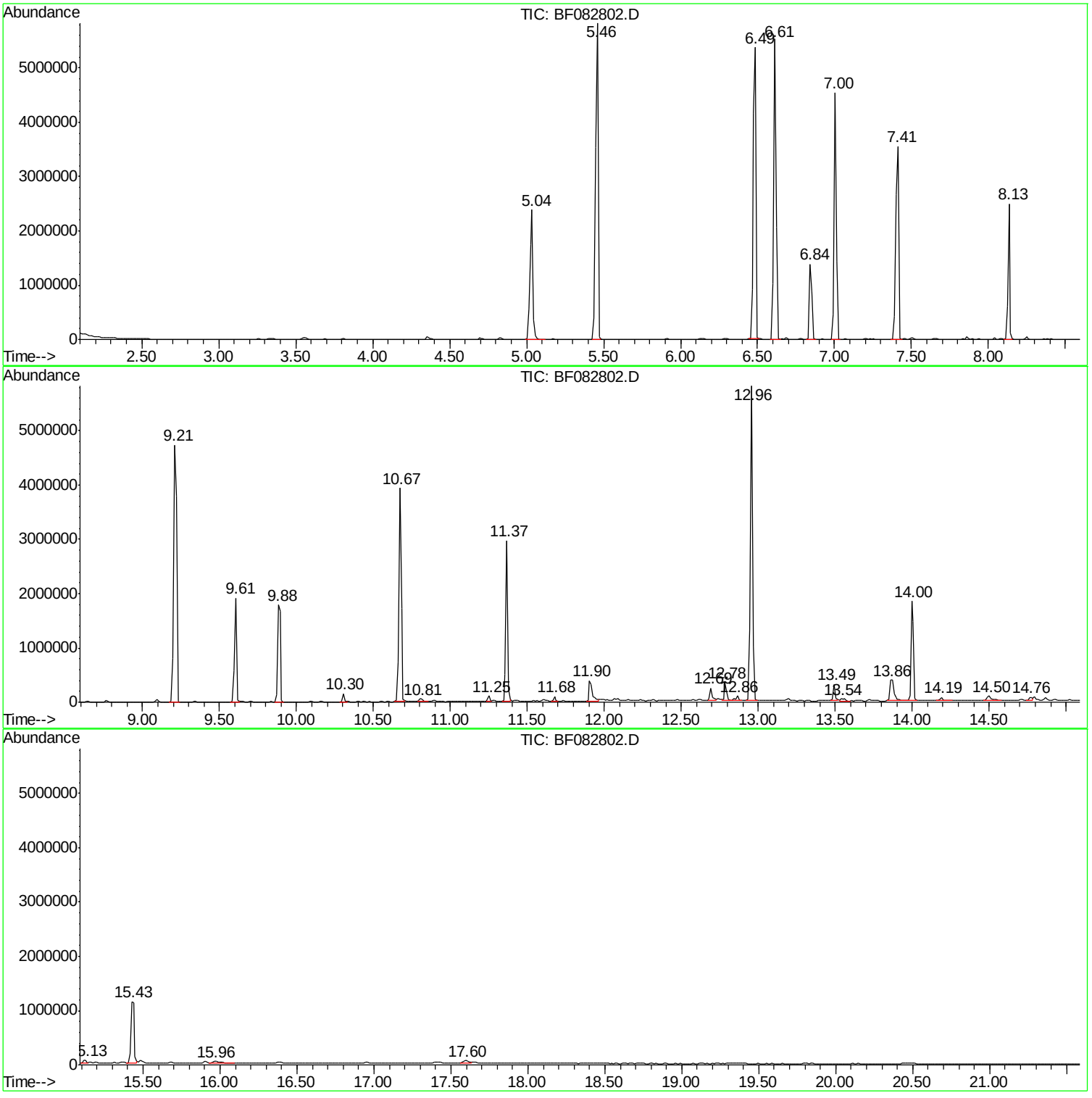
Sum of corrected areas: 66730383

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082802.D
Acq On : 7 Nov 2015 11:05
Operator : UM/IZ
Sample : G4246-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
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Operator : UM/IZ
Sample : G4246-06
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Instrument : BNA_F
ClientSampleId : T-12R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

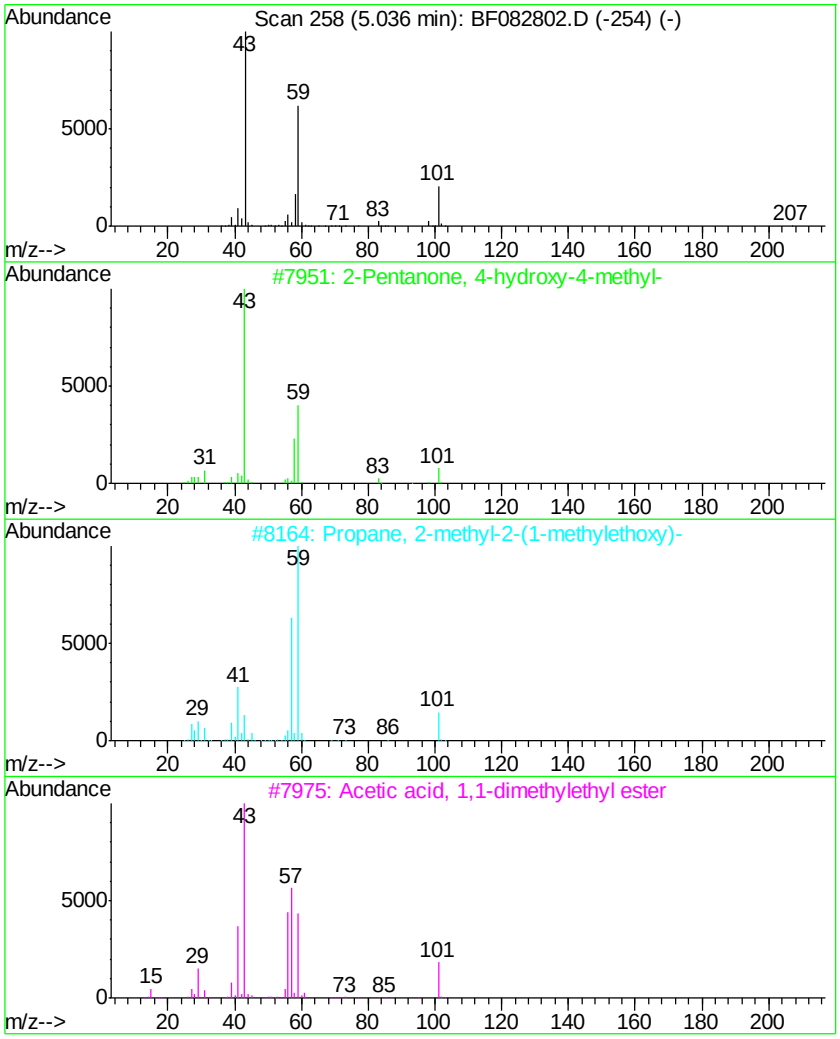
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

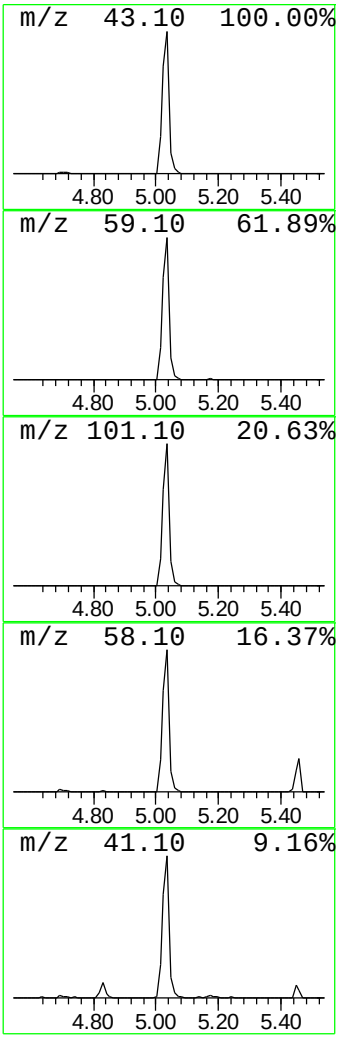
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	44.74 ng	3533040	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110815\
Data File : BF082802.D
Acq On : 7 Nov 2015 11:05
Operator : UM/IZ
Sample : G4246-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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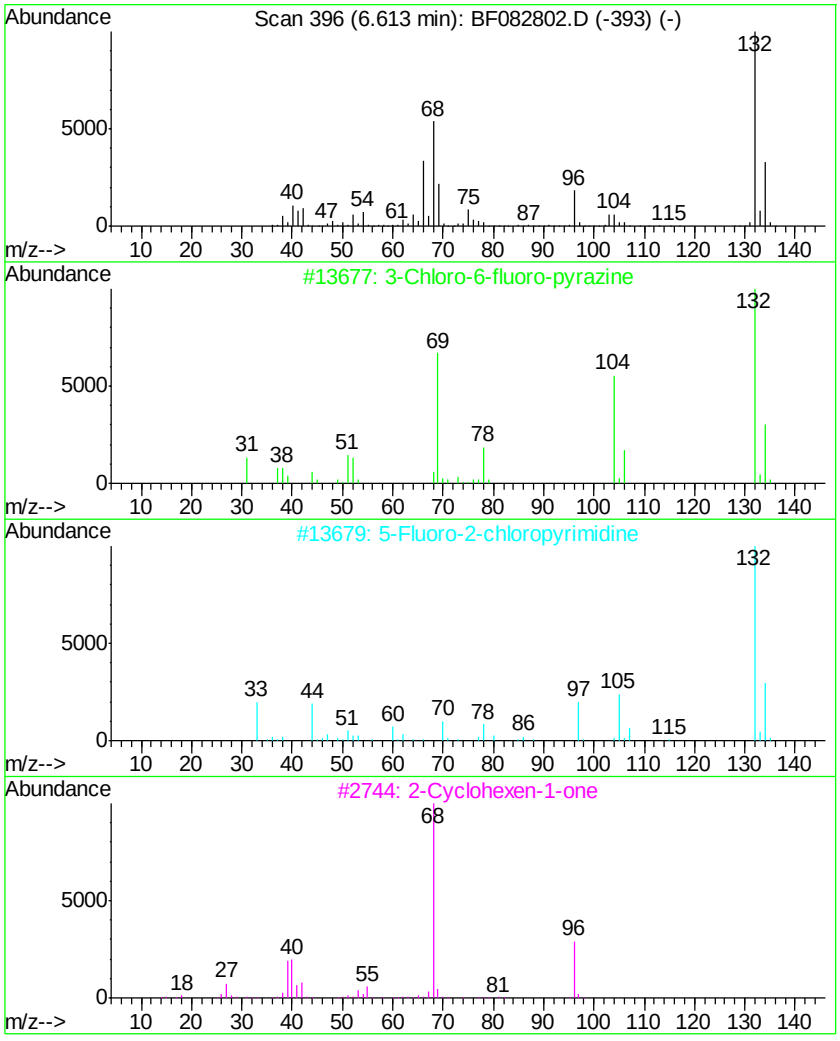
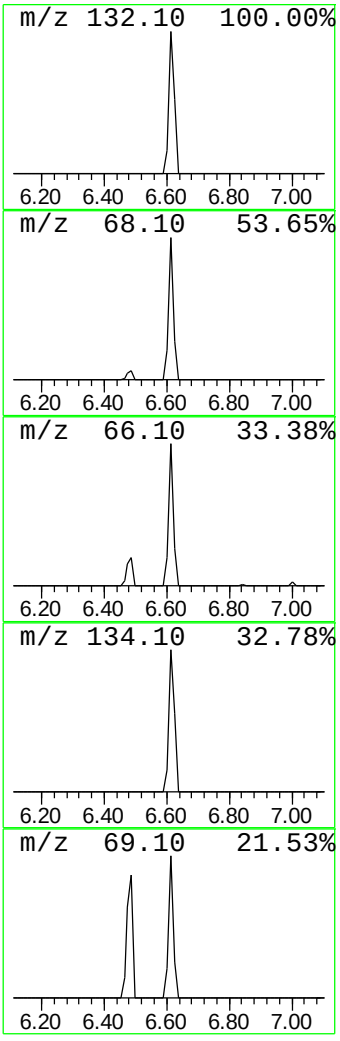
Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	74.86 ng	5911800	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9





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Operator : UM/IZ
Sample : G4246-06
Misc :
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Instrument : BNA_F
ClientSampleId : T-12R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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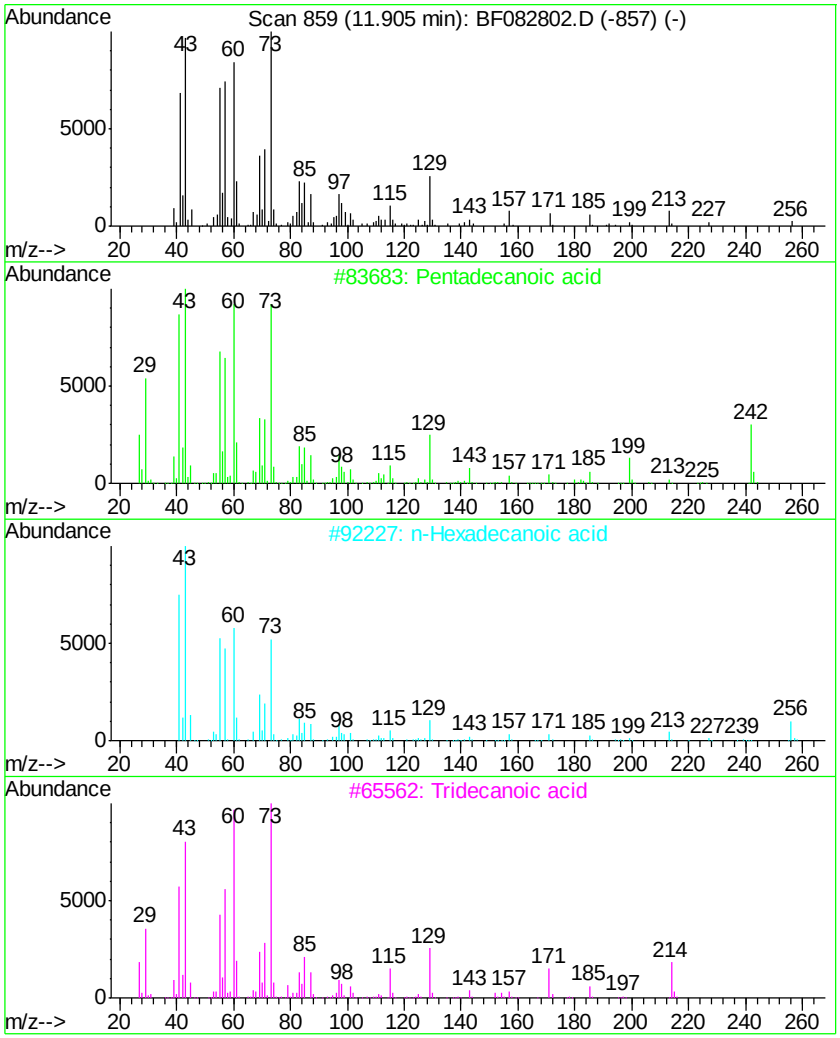
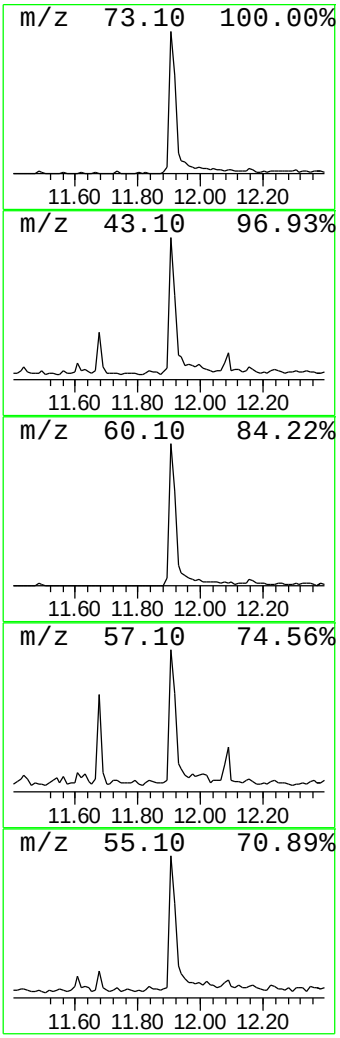
Peak Number 4 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	4.78 ng	604328	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	n-Decanoic acid	172	C10H20O2	000334-48-5	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Sample : G4246-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12R

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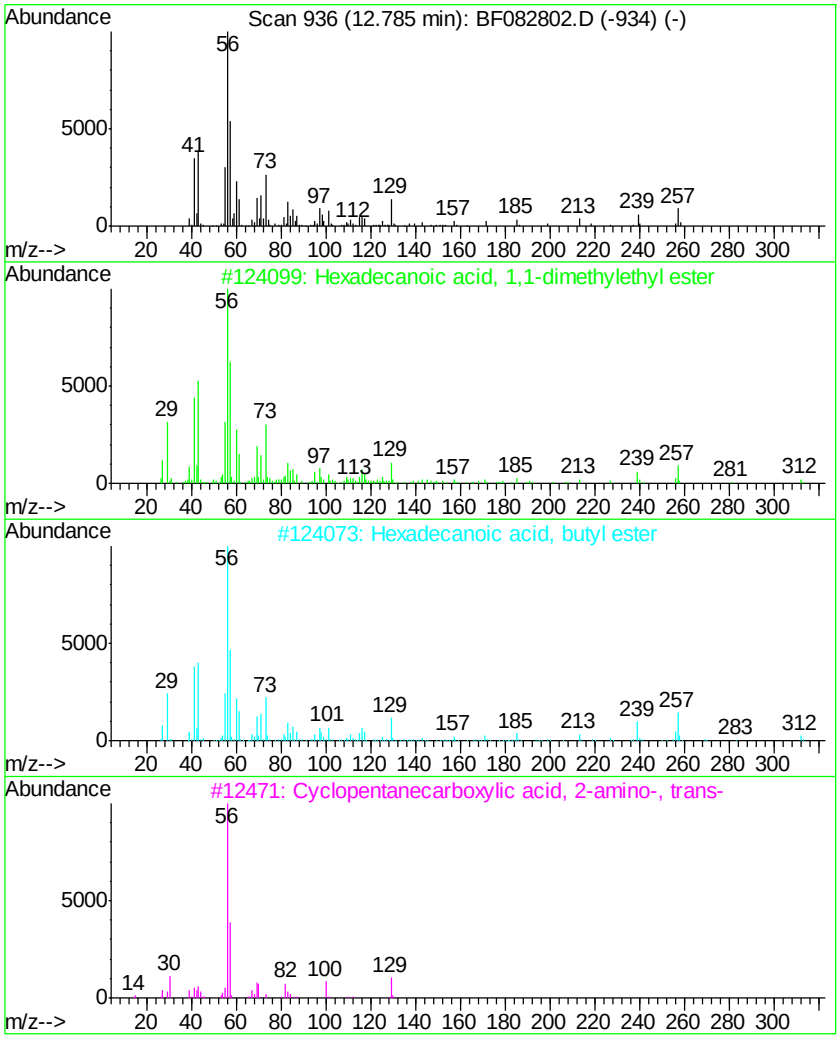
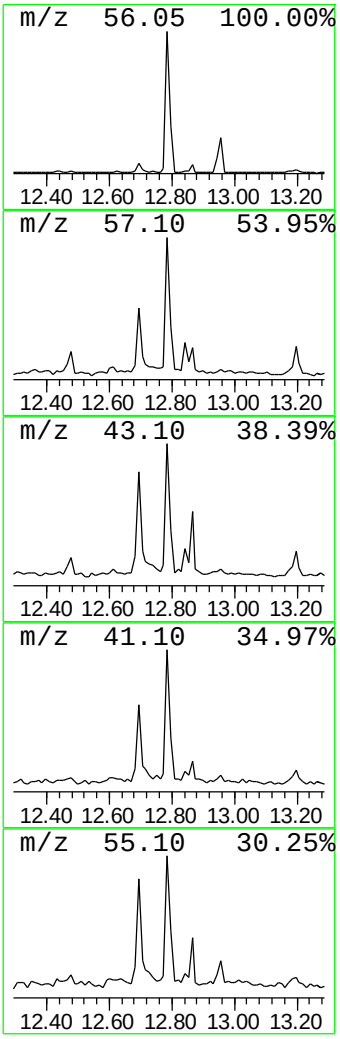
Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	3.10 ng	363812	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	43





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Sample : G4246-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-12R

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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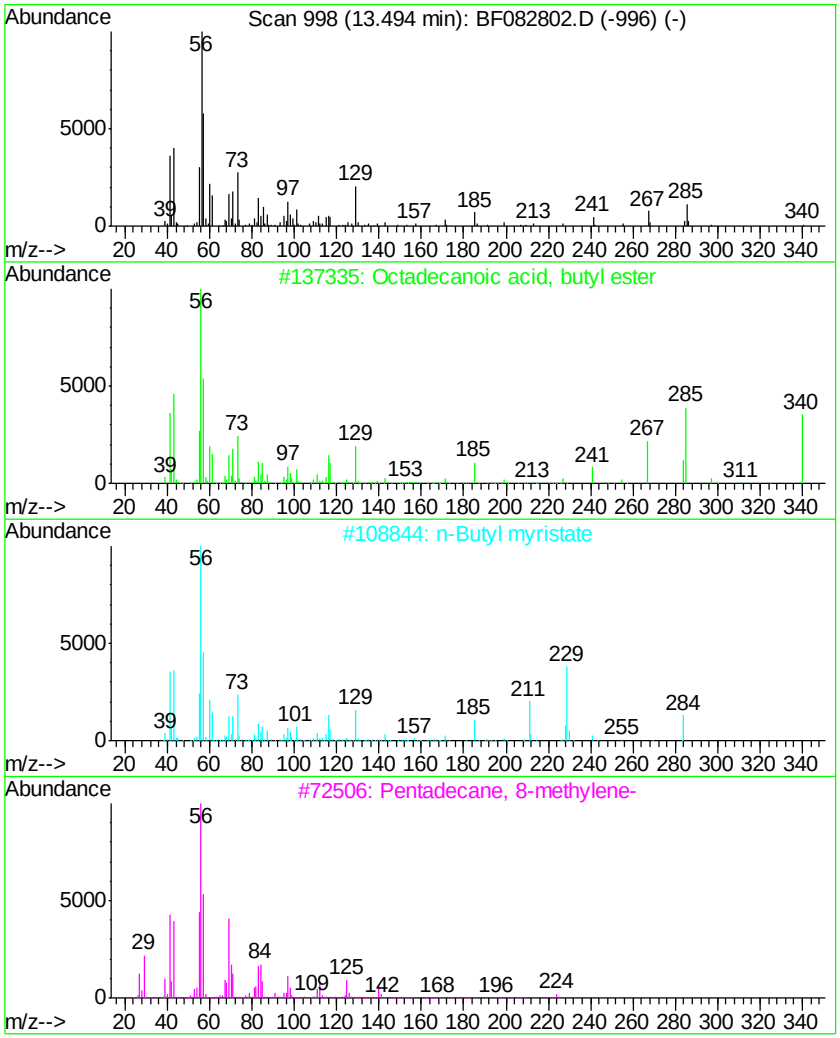
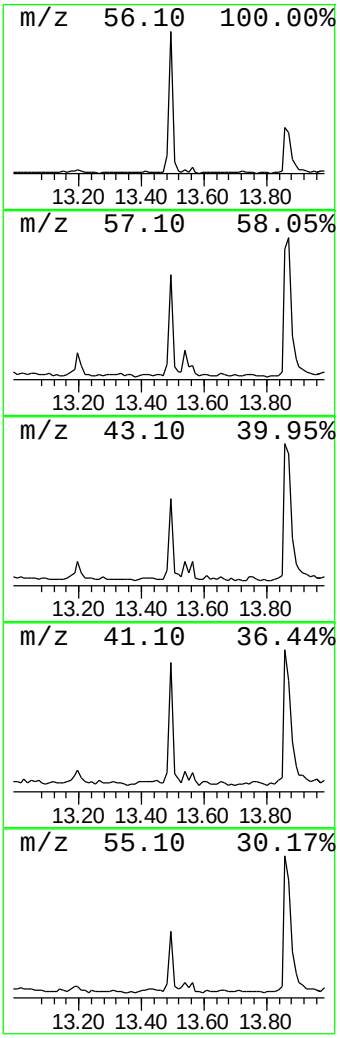
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.25 ng	264245	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	95
2	n-Butyl myristate	284	C18H36O2	000110-36-1	72
3	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	35
5	Cyclopentane, 3-hexyl-1,1-dimethyl-	182	C13H26	061142-65-2	32





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Sample : G4246-06
Misc :
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Instrument : BNA_F
ClientSampleId : T-12R

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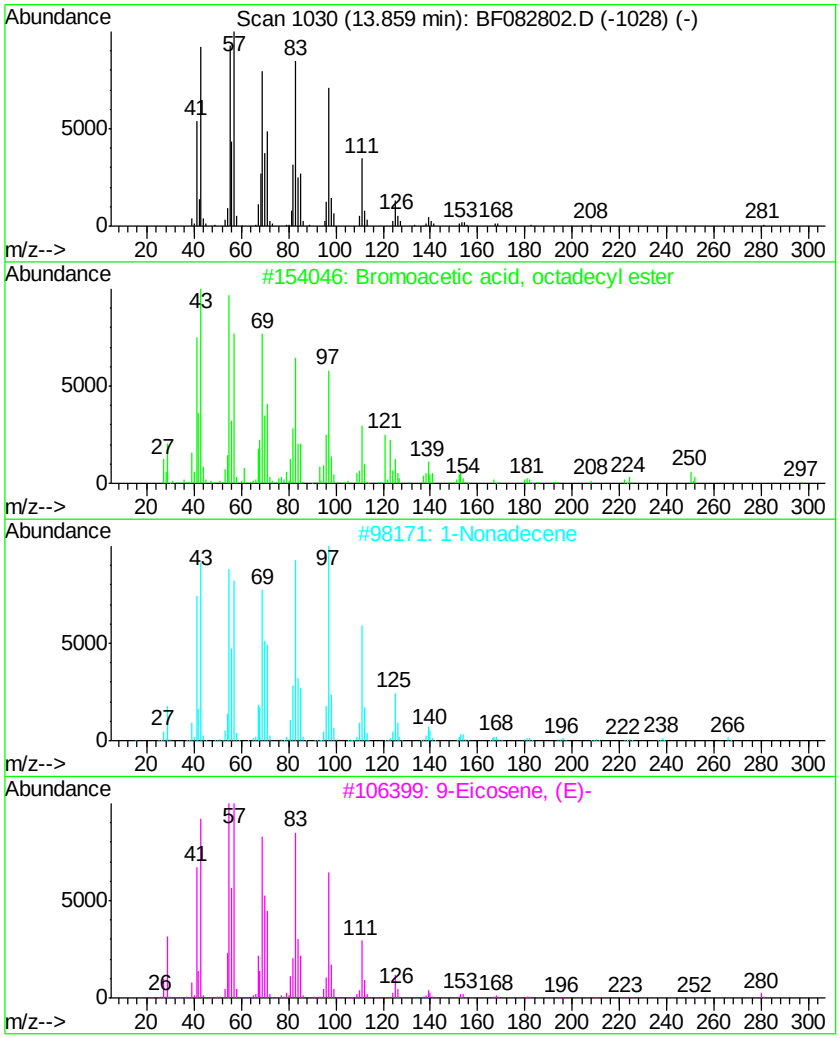
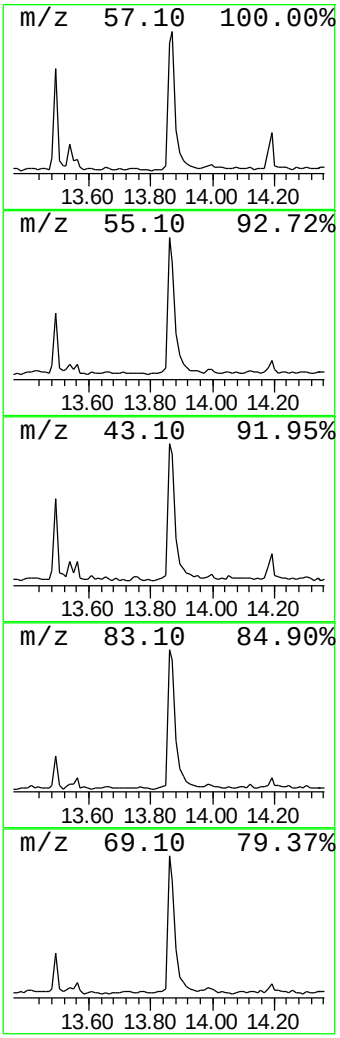
Peak Number 8 Bromoacetic acid, octadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	5.86 ng	688211	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	1-Octadecanol	270	C18H38O	000112-92-5	87
5	1-Hexadecanol	242	C16H34O	036653-82-4	87





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	44.7	ng	3533040	1	6.84	1579530	20.0
unknown6.61	6.61	74.9	ng	5911800	1	6.84	1579530	20.0
Pentadecanoic acid	11.90	4.8	ng	604328	4	11.37	2531100	20.0
Hexadecanoic acid...	12.79	3.1	ng	363812	5	14.00	2348180	20.0
Octadecanoic acid...	13.49	2.3	ng	264245	5	14.00	2348180	20.0
Bromoacetic acid,...	13.86	5.9	ng	688211	5	14.00	2348180	20.0